First principles simulations of structure and properties for complex systems

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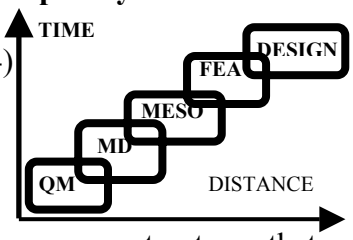

Many technologically important systems involve complex heterogeneous structures that make it difficult to determine the atomistic level structures needed for interpreting properties and designing new systems. For such systems small angle scattering (SAS) experiments (neutron or photon) sometimes provides the only structural information, but often many assumptions are required to invert the experimental data. First principles computational methods provide an attractive alternative to predict structures for complex systems, but it is often difficult to treat the size scales of interest at the time scales of interest. We will discuss some of the computational methods we have been using on such problems and some of the progress in applying these methods. Each case would greatly benefit from additional SAS experiments.

The applications to be described will be selected from:

- Structure and dynamics of supercooled and glassy water-sugar mixtures.
- Atomistic structure of and packing of Percec macromolecular dendrimer assemblies
- Structure, mechanical, and rheological properties of amorphous metals.
- Microstructure and dynamics of Nafion for PEM fuel cells.
- Atomistic structure of PAMAM macromolecular dendrimer assemblies
- Switching properties of Ferroelectric polymers
- Chemistry in reactive high energy materials under high stress conditions

In order to obtain first-principles treatments at long time scales and large distance scales we utilize multiscale strategies combining quantum mechanics (QM) to train reactive force fields, molecular dynamics (MD) using the reactive force fields to determine properties of intermediate sized systems, mesoscale force fields based on the atomistic MD useful for simulating systems at larger scales accessible to experiment, and extraction of continuum parameters and properties for macroscopic simulations and design.